sampled within supercell sizes accessible to present-day first-principles calculations. We address this challenge with a multiscale approach involving interatomic potentials that are parametrized and validated by density-functional theory. This allows to thoroughly sample the configuration space of $Li_4Ti_5O_{12}$ and perform an analysis of the variety of diffusion pathways. Particular focus is placed on the dependency of the average and local Li ion mobility on the thermodynamically accessible configuration space.

[1] B. Ziebarth *et al*, Phys. Rev. B **89**, 174301 (2014).

MM 14.7 Mon 17:30 H 0107

Self-Diffusion in Amorphous Silicon Investigated by Neutron Reflectometry — •Florian Strauss[1], Harald Schmidt[1], Jochen Stahn[2], and Thomas Geue[2] — [1]TU Clausthal, AG Mikrokinetik, Institut für Metallurgie, Deutschland — [2]Paul Scherrer Institut, Villigen, Schweiz

The characteristics of silicon self-diffusion in the amorphous state are still unknown, albeit the material is widely used in solar cells, flat screen displays and is looked at as a promising electrode material in Li-ion batteries. In this model system of a covalent amorphous semiconductor low diffusivities and intrinsic metastability necessitate the use of Neutron Reflectometry (NR) a method capable of determining diffusion lengths of 1 nm and below [1,2]. $^{29}Si/^{28}Si$ isotope multilayer structures are prepared by ion beam sputtering and thermally treated in an Ar atmosphere at temperatures up to 700 °C in order to induce isotope-interdiffusion. The chemical homogeneity and amorphous structure are confirmed by cross-sectional TEM measurements and XRD data. At temperatures between 350 and 500 °C a time dependent short range diffusion process on the length scale of 1 nm is observed and interpreted as a consequence of structural relaxation. At temperatures above 500 °C diffusion over a range of several nanometres is found. Additional measurements by Secondary Ion Mass Spectrometry confirm the data obtained by NR.

[1] H. Schmidt et al., Acta Mater. 56 (2008), 464
[2] E. Hüger et al., Appl. Phys. Lett. 93 (2008), 162104

MM 15: Hydrogen in metals III: Experiments

Time: Monday 15:45–18:00 Location: TC 006

Topical Talk MM 15.1 Mon 15:45 TC 006

On the combination of different experimental techniques to increase understanding on the hydrogen/material interaction in iron based alloys — Tom Depover, Elien Wallaert, Aurélie Laureys, Emilie Van den Eeckhout, and •Kim Verbeken — Ghent University, Department of Materials Science and Engineering, Technologiepark 903, B-9052 Ghent (Zwijnaarde)

Hydrogen induced cracking might arise when metals are in contact with an H-containing environment. Although known for a long time, the explanation of the responsible mechanism still remains under discussion. New, high strength metals appear more prone to H-related failure. The microstructure complexity of such metals even complicates the study of H induced phenomena. Moreover, H interacts in a very specific way with each microstructural feature. Furthermore, H-related research is a very challenging task due to the low H solubility, high H mobility and difficult H visualization.

H-material interactions can be studied via evaluating the effect of hydrogen on the mechanical properties, done by tensile tests after or during charging, characterizing H trapping via thermal desorption spectroscopy, studying H diffusion by electrochemical permeation and advanced characterization of H-induced cracks by electron backscatter diffraction. In this work, an overview is given on some recent results on the H-material interactions in iron-based alloys by combining these techniques. It will be demonstrated that the combination of these data is an asset contributing to the elucidation of the complicated H-material interactions.

MM 15.2 Mon 16:15 TC 006

Hydrogen diffusivity as a measure for relative dislocation densities in palladium — •Martin Deutges[1], Hans Peter Barth[2], Yuzeng Chen[3], Christine Borchers[1], and Reiner Kirchheim[1,4] — [1]Institut für Materialphysik, Georg-August Universität Göttingen — [2]Now at: DLR Göttingen — [3]State Key Lab of Solidification Processing, Northwestern Polytechnical University, Xi'an, P.R. China — [4]International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, Japan

It is well known that hydrogen affects the defect formation energy [1] which is thermodynamically described by the defactant concept [2]. The palladium-hydrogen system was chosen to analyze the effect of hydrogen on the formation of dislocations [3,4]. For this purpose palladium was loaded with different amounts of hydrogen and subsequently cold rolled. The dislocation density was quantified by measuring hydrogen diffusivity, which depends on the amount of trap sites for hydrogen. The results were compared to conventional XRD-methods [4]. After cold rolling, residual hydrogen is removed. During reloading with hydrogen the diffusion through the material is measured. The change in diffusivity allows to calculate the relative dislocation density. The presence of hydrogen during cold rolling of palladium leads to an increase of dislocation density [3].

[1] M. Deutges et al., Scripta Mater.68 (2013) 71.
[2] R. Kirchheim, Acta Mater. 55 (2007) 5129.
[3] Y.Z. Chen et al., Scripta Mater. 68 (2013) 743.
[4] M. Deutges et al., Acta Mater. 82 (2015) 266.

MM 15.3 Mon 16:30 TC 006

The impact of the carbon content on hydrogen diffusion and its influence on hydrogen embrittlement for lab-cast bainitic Fe-C steels — •Emilie Van den Eeckhout, Tom Depover, and Kim Verbeken — Department of Materials Science and Engineering, Ghent University (UGent), Technologiepark 903, B-9052 Ghent, Belgium

The present work investigates hydrogen diffusion in lab-cast alloys in which a bainitic microstructure was introduced. The high diffusivity of hydrogen is a critical factor affecting hydrogen induced cracking since hydrogen is enabled to diffuse to highly stressed regions, leading to an accelerated failure. When hydrogen diffusion is impeded by introducing hydrogen traps, fracture is delayed and the susceptibility to hydrogen embrittlement is reduced.

The hydrogen diffusion coefficient is calculated using a permeation cell based on the Devanathan - Stachurski permeability cell. Decreasing the carbon content from 0.4 to 0.2 wt. % elevates the hydrogen diffusion, which can be attributed to less hydrogen traps of the latter bainitic steel. The impact of this higher diffusivity on the degree of embrittlement was evaluated by performing tensile tests on in-situ hydrogen charged samples at various cross-head displacement speeds. A correlation with melt extraction tests is made to demonstrate the combined effect of hydrogen content and hydrogen diffusion on hydrogen embrittlement. Additionally, the role of hydrogen diffusion is evaluated by calculating and visualizing, by in-depth fractography, the distance hydrogen can diffuse during a tensile test.

15 min. break

MM 15.4 Mon 17:00 TC 006

HYDROGEN EMBRITTLEMENT IN AEROSPACE MATERIALS — •Sathiskumar Jothi, Nick Croft, and Stephen GR Brown — Swansea University, Swansea, UK

Microstructures play a prominent role in aerospace components which are typically made of high toughness, corrosion resistant and high strength structural polycrystalline metallic materials such as nickel and nickel based super alloys. Nickel and nickel based super alloys are made up of complex microstructures which are susceptible to delayed failure caused by absorption of hydrogen produced either during fabrication in manufacturing process (i.e electrodeposition, welding etc*) or during operational use under environmental conditions. Several catastrophic failures have occurred in nickel and nickel based super alloys due to intergranular as well transgranular hydrogen embrittlement (HE) and hydrogen stress cracking (HSC) not only in aerospace industries but also in many other engineering sectors. HE depends on many factors including hydrogen diffusion and segregation, microstructural morphology and defects, stresses and texture morphological behaviour. Under EU FP7 *MultiHy* project, we employed multiscale technique to investigate the influence of these factors in hydrogen embrittlement